WHAT IS CLAIMED IS:

1.   A method for preparing a virtual representation of a protein for in-silico processing, comprising:

        (1)   assessing the virtual representation of the protein for missing residues;

        (2)   modifying the virtual representation of the protein when a missing residue is detected;

        (3)   assessing the virtual representation of the protein for missing side chains;

        (4)   modifying the virtual representation of the protein when a missing side chain is detected; and

        (5)   outputting the modified virtual representation of the protein.

2.   The method according to claim 1, wherein step (1) comprises comparing a sequence listing of the protein with the virtual representation of the protein to determine whether any residues listed in the sequence listing are missing from the virtual representation of the protein.

3.   The method according to claim 1, wherein step (1) comprises examining entries in a residue-number column of a protein database file for missing numbers.

4.   The method according to claim 1, wherein step (1) comprises examining a header section of the virtual representation of the protein for an identification of residues missing from the virtual representation of the protein.

5.   The method according to claim 1, wherein step (3) comprises comparing a portion of the virtual representation of the protein with a template.

6.   The method according to claim 1, wherein step (4) comprises identifying multiple solutions for a missing side chain and modifying the virtual representation of the protein with a selected one of the multiple solutions.

7.   The method according to claim 1, further comprising:

        (1)   assessing the virtual representation of the protein for atoms that are not part of the protein; and

        (2)   modifying the virtual representation of the protein when an atom that is not part of the protein is identified.

8.   The method according to claim 7, wherein step (2) comprises removing an atom that is not part of the protein from the virtual representation of the protein.

9.   The method according to claim 1, further comprising:

        (1)   assessing the virtual representation of the protein for hydrogen atom sites; and

        (2)   modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified.

10.   The method according to claim 9, wherein step (2) comprises assigning initial coordinates to the hydrogen atom.

11.   The method according to claim 10, wherein step (2) further comprises determining an orientation of the hydrogen atom and modifying the initial coordinates to correspond to the orientation.

12.   The method according to claim 11, wherein step (2) further comprises selecting the orientation of the hydrogen atom from a look-up table.

13.   The method according to claim 11, wherein step (2) further comprises determining the orientation of the hydrogen atom present on the side chain of a residue using a search and evaluation process, wherein the conformation of the functional group associated with the hydrogen atom is sampled to determine a low energy conformation.

14.   The method according to claim 13, wherein step (2) further comprises determining the orientation of the hydrogen atom using a simulated annealing process.

15.   The method according to claim 14, wherein the simulated annealing process calculates the coordinates of the hydrogen atom that provide a relatively low energy state for the residue.

16.   The method according to claim 14, wherein the simulated annealing process receives as input information relating to features that are relatively near to the hydrogen atom.

17.   The method according to claim 9, further comprisingassigning a protonation state to the residue.

18.   The method according to claim 9, further comprising:

        (1)   determining if the partial charges or electron distribution of one or more regions of the protein must be recalculated; and

        (2)   optionally assigning and/or modifying the partial charges or electron distribution of one or more regions of the protein.

19.   The method according to claim 1, further comprising:

        (1)   assessing an energy state of the virtual representation of the protein; and

(2)   modifying the virtual representation of the protein to reduce the energy state.

20.   The method according to claim 1, further comprising:

(1)   assessing a structural quality of the virtual representation of the protein;

(2)   assessing a structural quality of the modified virtual representation of the protein;

(3)   comparing the structural quality assessments of steps (1) and (2); and

(4)   replacing the virtual representation of the protein with the modified virtual representation of the protein when the structural quality of the modified virtual representation of the protein is better than the structural quality of the virtual representation of the protein.

21.   The method according to claim 1, wherein at least a portion of one or more of steps (1) through (4) are performed in a computer system under control of a computer program.

22.   The method according to claim 1, wherein at least a portion of one or more of steps (1) through (4) are performed in a computer system under control of a computer program based on input received from a user.

23.   The method according to claim 1, further comprising minimizing an energy level of the virtual representation of the protein.

24.   The method according to claim 1, further comprising minimizing the energy level of a portion of the virtual representation of the protein.

25.   The method according to claim 1, further comprising minimizing the energy level of a binding site of the virtual representation of the protein.

26.   The method according to claim 25, further comprising minimizing the energy level of the binding site including a virtual representation of a small molecule coupled to the binding site.

27.   The method according to claim 26, further comprising minimizing the energy level of the binding site including a virtual representation of a peptide coupled to the binding site.

28.   The method according to claim 1, further comprising mutating a residue of the virtual representation of the protein.

29.   A system for preparing a virtual representation of a protein for in-silico processing, comprising:

a database for storing a virtual representation of the protein;

a virtual representation engine for accessing and modifying the virtual representation of the protein to produce a modified virtual presentation of the protein; and

an output module for outputting the modified virtual presentation of the protein;

wherein the virtual representation engine assesses the virtual representation of the protein for missing residues and modifies the virtual representation of the protein when a missing residue is detected; and

wherein the virtual representation engine assesses the virtual representation of the protein for missing side chains and modifies the virtual representation of the protein when a missing side chain is detected.

30.   The system according to claim 29, wherein the virtual representation engine assessing the virtual representation of the protein for missing residues comprises comparing a sequence listing of the protein with the virtual

representation of the protein to determine whether any residues listed in the sequence listing are missing from the virtual representation of the protein.

31. The system according to claim 29, wherein the virtual representation engine assessing the virtual representation of the protein for missing residues comprises examining entries in a residue-number column of a protein database file for missing numbers.

32. The system according to claim 29, wherein the virtual representation engine assessing the virtual representation of the protein for missing residues comprises examining a header section of the virtual representation of the protein for an identification of residues missing from the virtual representation of the protein.

33. The system according to claim 29, wherein the virtual representation engine assessing the virtual representation of the protein for missing side chains comprises comparing a portion of the virtual representation of the protein with a template.

34. The system according to claim 29, wherein the virtual representation engine modifying the virtual representation of the protein when a missing side chain is detected comprises identifying multiple solutions for a missing side chain and modifying the virtual representation of the protein with a selected one of the multiple solutions.

35. The system according to claim 29, further comprising the virtual representation engine assesses the virtual representation of the protein for atoms that are not part of the protein and modifies the virtual representation of the protein when an atom that is not part of the protein is identified.

36. The system according to claim 35, wherein the virtual representation engine modifying the virtual representation of the protein when an atom that is not part of the protein is identified comprises removing an atom that is not part of the protein from the virtual representation of the protein.

37. The system according to claim 29, further comprising the virtual representation engine assesses the virtual representation of the protein for hydrogen atom sites and modifies the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified.

38. The system according to claim 37, wherein the virtual representation engine modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified comprises assigning initial coordinates to the hydrogen atom.

39. The system according to claim 38, wherein the virtual representation engine modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified further comprises determining an orientation of the hydrogen atom and modifying the initial coordinates to correspond to the orientation.

40. The system according to claim 39, wherein the virtual representation engine modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified further comprises selecting the orientation of the hydrogen atom from a look-up table.

41. The system according to claim 39, wherein the virtual representation engine modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified further comprises determining the orientation of the hydrogen atom using a search and evaluation process.

42. The system according to claim 41, wherein the virtual representation engine modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified further comprises determining the orientation of the hydrogen atom using a simulated annealing process.

43. The system according to claim 42, wherein the simulated annealing process calculates the coordinates of the hydrogen atom that provide a relatively low energy state for the residue.

44. The system according to claim 42, wherein the simulated annealing process receives input information relating to features that are relatively near to the hydrogen atom.

45. The system according to claim 37, wherein the virtual representation engine assigns a protonation state to the residue.

46. The system according to claim 29, wherein the virtual representation engine assesses an energy state of the virtual representation of the protein and modifies the virtual representation of the protein to reduce the energy state.

47. The system according to claim 29, further comprising:

wherein the virtual representation engine assesses a structural quality of the virtual representation of the protein and accesses a structural quality of the modified virtual representation of the protein,

wherein the virtual representation engine further compares the structural quality assessments of the virtual representation of the protein and of the modified virtual representation of the protein, and

wherein the virtual representation engine replaces the virtual representation of the protein with the modified virtual representation of the protein when the structural quality of the modified virtual representation of the protein is better than the structural quality of the virtual representation of the protein.

48.   The system according to claim 29, wherein at least a portion of one or more of the virtual representation engine assessing the virtual representation of the protein for missing residues, the virtual representation engine modifying the virtual representation of the protein when a missing residue is detected, the virtual representation engine assessing the virtual representation of the protein for missing side chains and the virtual representation engine modifying the virtual representation of the protein when a missing side chain is detected are performed in a computer system under control of a computer program.

49.   The system according to claim 29, wherein at least a portion of the virtual representation engine assessing the virtual representation of the protein for missing residues, the virtual representation engine modifying the virtual representation of the protein when a missing residue is detected, the virtual representation engine assessing the virtual representation of the protein for missing side chains and the virtual representation engine modifying the virtual representation of the protein when a missing side chain is detected are performed in a computer system under control of a computer program based on input received from a user.

50.   The system according to claim 29, further comprising the virtual representation engine minimizing an energy level of the virtual representation of the protein.

51.   The system according to claim 50, further comprising the virtual representation engine minimizing the energy level of a portion of the virtual representation of the protein.

52.   The system according to claim 51, further comprising the virtual representation engine minimizing the energy level of a binding site of the virtual representation of the protein.

53.   The system according to claim 52, further comprising the virtual representation engine minimizing the energy level of the binding site including a virtual representation of a small molecule coupled to the binding site.

54.   The system according to claim 53, further comprising the virtual representation engine minimizing the energy level of the binding site including a virtual representation of a peptide coupled to the binding site.

55.   The system according to claim 29, further comprises the virtual representation engine mutates a residue of the virtual representation of the protein.

56.   A computer program product including a computer useable medium having computer program logic stored therein to enable a computer system to prepare a virtual representation of a protein for in-silico processing, wherein said computer program logic comprises:
        a first function that causes the computer system to assess the virtual representation of the protein for missing residues;
        a second function that causes the computer system to modify the virtual representation of the protein when a missing residue is detected;
        a third function that causes the computer system to assess the virtual representation of the protein for missing side chains; and

a fourth function that causes the computer system to modify the virtual representation of the protein when a missing side chains is detected.

57.   The computer program product according to claim 56, wherein the first function that causes the computer system to assess comprises comparing a sequence listing of the protein with the virtual representation of the protein to determine whether any residues listed in the sequence listing are missing from the virtual representation of the protein.

58.   The computer program product according to claim 56, wherein the first function that causes the computer system to assess comprises examining entries in a residue-number column of a protein database file for missing numbers.

59.   The computer program product according to claim 56, wherein the first function that causes the computer system to assess comprises examining a header section of the virtual representation of the protein for an identification of residues missing from the virtual representation of the protein.

60.   The computer program product according to claim 56, wherein the third function that causes the computer system to assess comprises comparing a portion of the virtual representation of the protein with a template.

61.   The computer program product according to claim 56, wherein the fourth function that causes the computer system to modify comprises identifying multiple solutions for a missing side chain and modifying the virtual representation of the protein with a selected one of the multiple solutions.

62.   The computer program product according to claim 56, wherein the computer program logic further comprises:

a fifth function that causes the computer system to assess the virtual representation of the protein for atoms that are not part of the protein; and

a sixth function that causes the computer system to modify the virtual representation of the protein when an atom that is not part of the protein is identified

63. The computer program product according to claim 62, wherein the sixth function that causes the computer system to modify comprises removing an atom that is not part of the protein from the virtual representation of the protein.

64. The computer program product according to claim 56, wherein the computer program logic further comprises:

a fifth function that causes the computer system to assess the virtual representation of the protein for hydrogen atom sites; and

a sixth function that causes the computer system to modify the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified.

65. The computer program product according to claim 62, wherein the sixth function that causes the computer system to modify comprises assigning initial coordinates to the hydrogen atom.

66. The computer program product according to claim 65, wherein the sixth function that causes the computer system to modify further comprises determining an orientation of the hydrogen atom and modifying the initial coordinates to correspond to the orientation.

67. The computer program product according to claim 66, wherein the sixth function that causes the computer system to modify further comprises selecting the orientation of the hydrogen atom from a look-up table.

68.   The computer program product according to claim 66, wherein the sixth function that causes the computer system to modify further comprises determining the orientation of the hydrogen atom using a search and evaluation process.

69.   The computer program product according to claim 68, wherein the sixth function that causes the computer system to modify further comprises determining the orientation of the hydrogen atom using a simulated annealing process.

70.   The computer program product according to claim 69, wherein the simulated annealing process calculates the coordinates of the hydrogen atom that provide a relatively low energy state for the residue.

71.   The computer program product according to claim 69, wherein the simulated annealing process receives as input information relating to features that are relatively near to the hydrogen atom.

72.   The computer program product according to claim 64, wherein the computer program logic further comprises:
        a seventh function that causes the computer system to assign a protonation state to the residue.

73.   The computer program product according to claim 56, wherein the computer program logic further comprises:
        a fifth function that causes the computer system to assess an energy state of the virtual representation of the protein; and
        a sixth function that causes the computer system to modify the virtual representation of the protein to reduce the energy state.

74.   The computer program product according to claim 56, wherein the computer program logic further comprises:

     a fifth function that causes the computer system to assess a structural quality of the virtual representation of the protein;

     a sixth function that causes the computer system to assess a structural quality of the modified virtual representation of the protein;

     a seventh function that causes the computer system to compare the structural quality assessments of the fifth function and the sixth function; and

     an eighth function that causes the computer system to replace the virtual representation of the protein with the modified virtual representation of the protein when the structural quality of the modified virtual representation of the protein is better than the structural quality of the virtual representation of the protein.

75.   The computer program product according to claim 56, wherein at least a portion of one or more of functions one through four are performed in a computer system under control of a computer program.

76.   The computer program product according to claim 56, wherein at least a portion of one or more of functions one through four are performed in a computer system under control of a computer program based on input received from a user.

77.   The computer program product according to claim 56, further comprising a fifth function that causes a computer system to minimize an energy level of the virtual representation of the protein.

78.   The computer program product according to claim 77, further comprising a sixth function that causes a computer system to minimize the energy level of a portion of the virtual representation of the protein.

79.   The computer program product according to claim 78, further comprising a seventh function that causes a computer system to minimize the energy level of a binding site of the virtual representation of the protein.

80.   The computer program product according to claim 79, further comprising an eighth function that causes a computer system to minimize the energy level of the binding site of including a virtual representation of a small molecule coupled to the binding site.

81.   The computer program product according to claim 80, further comprising a ninth function that causes a computer system to minimize the energy level of the binding site including a virtual representation of a peptide coupled to the binding site.

82.   The computer program product according to claim 56, further comprising a fifth function that causes a computer system to mutate a residue of the virtual representation of the protein.

83.   The computer program product according to claim 56, further comprising a fifth function that causes a computer system to output the modified virtual representation of the protein.

84.   An apparatus for preparing a virtual representation of a protein for in-silico processing, comprising:

        means for assessing the virtual representation of the protein for missing residues;

        means for modifying the virtual representation of the protein when a missing residue is detected;

        means for assessing the virtual representation of the protein for missing side chains; and

means for modifying the virtual representation of the protein when a missing side chains is detected.

85.   The apparatus according to claim 84, wherein the means for assessing the virtual representation of the protein for missing residues comprises means for comparing a sequence listing of the protein with the virtual representation of the protein to determine whether any residues listed in the sequence listing are missing from the virtual representation of the protein.

86.   The apparatus according to claim 84, wherein the means for assessing the virtual representation of the protein for missing residues comprises means for examining entries in a residue-number column of a protein database file for missing numbers.

87.   The apparatus according to claim 84, wherein the means for assessing the virtual representation of the protein for missing residues comprises means for examining a header section of the virtual representation of the protein for an identification of residues missing from the virtual representation of the protein.

88.   The apparatus according to claim 84, wherein the means for assessing the virtual representation of the protein for missing side chains comprises means for comparing a portion of the virtual representation of the protein with a template.

89.   The apparatus according to claim 84, wherein the means for modifying the virtual representation of the protein when a missing side chains is detected comprises:

        means for identifying multiple solutions for a missing side chain; and

        means for modifying the virtual representation of the protein with a selected one of the multiple solutions.

90.   The apparatus according to claim 84, further comprising:

means for assessing the virtual representation of the protein for atoms that are not part of the protein; and

means for modifying the virtual representation of the protein when an atom that is not part of the protein is identified

91.   The apparatus according to claim 90, wherein the means for modifying the virtual representation of the protein when an atom that is not part of the protein is identified comprises means for removing an atom that is not part of the protein from the virtual representation of the protein.

92.   The apparatus according to claim 84, further comprising:

means for assessing the virtual representation of the protein for hydrogen atom sites; and

means for modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified.

93.   The apparatus according to claim 92, wherein the means for modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified comprises means for assigning initial coordinates to the hydrogen atom.

94.   The apparatus according to claim 93, wherein the means for modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified further comprises:

means for determining an orientation of the hydrogen atom; and

means for modifying the initial coordinates to correspond to the orientation.

95.   The apparatus according to claim 94, wherein the means for modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified further comprises means for selecting the orientation of the hydrogen atom from a look-up table.

96.   The apparatus according to claim 94, wherein the means for modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified further comprises means for determining the orientation of the hydrogen atom using a search and evaluation process.

97.   The apparatus according to claim 96, wherein the means for modifying the virtual representation of the protein to include a hydrogen atom when a hydrogen atom site is identified further comprises means for determining the orientation of the hydrogen atom using a simulated annealing process.

98.   The apparatus according to claim 97, wherein the simulated annealing process calculates the coordinates of the hydrogen atom that provide a relatively low energy state for the residue.

99.   The apparatus according to claim 97, wherein the simulated annealing process receives as input information relating to features that are relatively near to the hydrogen atom.

100.   The apparatus according to claim 92, further comprising means for assigning a protonation state to a residue.

101.   The apparatus according to claim 84, further comprising:
        means for assessing an energy state of the virtual representation of the protein; and

means for modifying the virtual representation of the protein to reduce the energy state.

102. The apparatus according to claim 84, further comprising:

means for assessing a structural quality of the virtual representation of the protein;

means for assessing a structural quality of the modified virtual representation of the protein;

means for comparing the structural quality assessments of the means for assessing a structural quality of the virtual representation of the protein and the means for assessing a structural quality of the modified virtual representation of the protein; and

means for replacing the virtual representation of the protein with the modified virtual representation of the protein when the structural quality of the modified virtual representation of the protein is better than the structural quality of the virtual representation of the protein.

103. The apparatus according to claim 84, wherein at least a portion of one or more of the means for assessing the virtual representation of the protein for missing residues, the means for modifying the virtual representation of the protein when a missing residue is detected, the means for assessing the virtual representation of the protein for missing side chains, and the means for modifying the virtual representation of the protein when a missing side chains is detected are performed in a computer system under control of a computer program.

104. The apparatus according to claim 84, wherein at least a portion of one or more of the means for assessing the virtual representation of the protein for missing residues, the means for modifying the virtual representation of the protein when a missing residue is detected, the means for assessing the virtual representation of the protein for missing side chains, and the means for

modifying the virtual representation of the protein when a missing side chains is detected are performed in a computer system under control of a computer program based on input received from a user.

105. The apparatus according to claim 84, further comprising means for minimizing an energy level of the virtual representation of the protein.

106. The apparatus according to claim 105, further comprising means for minimizing the energy level of a portion of the virtual representation of the protein.

107. The apparatus according to claim 106, further comprising means for minimizing the energy level of a binding site of the virtual representation of the protein.

108. The apparatus according to claim 107, further comprising means for minimizing the energy level of the binding site of including a virtual representation of a small molecule coupled to the binding site.

109. The apparatus according to claim 108, further comprising means for minimizing the energy level of the binding site including a virtual representation of a peptide coupled to the binding site.

110. The apparatus according to claim 84, further comprising means for mutating a residue of the virtual representation of the protein.

111. The apparatus according to claim 84, further comprising means for outputting the modified virtual representation of the protein.

112.   A method for preparing a virtual representation of a protein for in-silico processing, comprising the steps of:

(1)   assessing the virtual representation of the protein for missing residues;

(2)   modifying the virtual representation of the protein when a missing residue is detected;

(3)   assessing the virtual representation of the protein for missing side chains;

(4)   modifying the virtual representation of the protein when a missing side chain is detected;

(5)   assessing the virtual representation of the protein for atoms that are not part of the protein;

(6)   modifying the virtual representation of the protein when an atom that is not part of the protein is identified

(7)   assessing the virtual representation of the protein for hydrogen atom sites;

(8)   modifying the virtual representation of the protein to include hydrogen atoms at the hydrogen atom sites;

(9)   assigning initial coordinates to the hydrogen atoms; and

(10)   modifying the virtual representation of the protein to include protonation states for the residue.

113.   A system for preparing a virtual representation of a protein for in-silico processing, comprising:

a database for storing a virtual representation of the protein;

a virtual representation engine for accessing and modifying the virtual representation of the protein to produce a modified virtual presentation of the protein; and

an output module for displaying the modified virtual presentation of the protein;

wherein the virtual representation engine assesses the virtual representation of the protein for missing residues and modifies the virtual representation of the protein when a missing residue is detected;

wherein the virtual representation engine assesses the virtual representation of the protein for missing side chains and modifies the virtual representation of the protein when a missing side chain is detected;

wherein the virtual representation engine assesses the virtual representation of the protein for atoms that are not part of the protein and modifies the virtual representation of the protein when an atom that is not part of the protein is identified;

wherein the virtual representation engine assesses the virtual representation of the protein for hydrogen atom sites and modifies the virtual representation of the protein to include hydrogen atoms at the hydrogen atom sites; and

wherein the virtual representation engine assigns initial coordinates to the hydrogen atoms and modifies the virtual representation of the protein to include protonation states for the residue.

114. A computer program product including a computer useable medium having computer program logic stored therein to enable a computer system to prepare a virtual representation of a protein for *in-silico* processing, where the computer program logic comprises:

a first function that causes the computer system to assess the virtual representation of the protein for missing residues;

a second function that causes the computer system to modify the virtual representation of the protein when a missing residue is detected;

a third function that causes the computer system to assess the virtual representation of the protein for missing side chains;

a fourth function that causes the computer system to modify the virtual representation of the protein when a missing side chain is detected;

a fifth function that causes the computer system to assess the virtual representation of the protein for atoms that are not part of the protein;

a sixth function that causes the computer system to modify the virtual representation of the protein when an atom that is not part of the protein is identified

a seventh function that causes the computer system to assess the virtual representation of the protein for hydrogen atom sites;

an eighth function that causes the computer system to modify the virtual representation of the protein to include hydrogen atoms at the hydrogen atom sites;

a ninth function that causes the computer system to assign initial coordinates to the hydrogen atoms; and

a tenth function that causes the computer system to modify the virtual representation of the protein to include protonation states for the residue.

115.   An apparatus for preparing a virtual representation of a protein for *in-silico* processing, comprising:

means for assessing the virtual representation of the protein for missing residues;

means for modifying the virtual representation of the protein when a missing residue is detected;

means for assessing the virtual representation of the protein for missing side chains;

means for modifying the virtual representation of the protein when a missing side chain is detected;

means for assessing the virtual representation of the protein for atoms that are not part of the protein;

means for modifying the virtual representation of the protein when an atom that is not part of the protein is identified

means for assessing the virtual representation of the protein for hydrogen atom sites;

means for modifying the virtual representation of the protein to include hydrogen atoms at the hydrogen atom sites;

means for assigning initial coordinates to the hydrogen atoms; and

means for modifying the virtual representation of the protein to include protonation states for the residue.